MCCI and Ducted Fuel Injection (Part 2)

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Project # FT078

FY19 DOE Vehicle Technologies Office
Annual Merit Review
better fuels | better vehicles | sooner
Overview

Four Projects

- E.2.2.8 - Catalyst light-off and cold-start emissions (Wissink)
- E.2.2.9 - Catalyst heating operation (Busch)
- G.2.18 - Effect of Fuel Properties on In-nozzle Cavitation (Som)
- E.1.4.1 - X-ray Measurements of Injection and Mixture Formation (Powell)

Timeline

- All projects new in FY2019
- Projects end after FY2021

Budget

- CN and Cold Start: $222k
- Oxy Fuels and Cold Start: $160k
- Cavitation Modeling: $120k
- Cavitation Measurements: $155k

Collaboration

- Catalysts: Ford, Daimler
- Cavitation: Powell, Som, Pickett, ECN, Co-Optima Fuels Team

Barriers

- Understand and improve combustion during cold start to reduce emissions
- Provide a comprehensive understanding of fuel sprays with support from advanced diagnostics and high-fidelity modeling tools
- A comprehensive understanding of fuel sprays, combustion, and emissions formation is needed to develop optimal combustion system designs
Develop a fundamental understanding of the relationship between fuel properties and emissions

In-Cylinder Emissions Reduction (sprays, mixture formation)
- Cavitation Modeling, Cavitation Measurements
- Cavitation and erosion alter injection and combustion, and depend on the physical properties of the fuel

In-Cylinder Effects on Emissions Control (catalyst heating, cold start)
- CN and Cold Start, Oxy Fuels and Cold Start
- Fuel properties impact combustion, emissions, and aftertreatment performance
In-cylinder emissions reduction requires detailed knowledge of fuel effects on injection and mixture formation

- **Objective**: Perform nozzle flow measurements and simulations to characterize the influence of critical fuel properties on cavitation. Identify fuel properties that increase cavitation and erosion.
- **Impact**: Improved fundamental understanding of cavitation and erosion. Integrate a new cavitation erosion model into a computational screening tool for new fuels.

Decreasing emissions at cold start requires either decreased engine-out emissions, or faster catalyst light-off

- **Objective**: Assess the ability of cetane number to increase exhaust temperature
- **Objective**: Assess the ability of oxygenated fuels to lower HC emissions
- **Impact**: Improved understanding of how fuel properties can be manipulated in order to decrease emissions under cold start conditions
<table>
<thead>
<tr>
<th>Month / Year</th>
<th>Description of Milestone or Go/No-Go Decision</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>March 2019</td>
<td><strong>Oxy Fuels &amp; Cold Start:</strong> GO/NOGO: Assess infrared in-cylinder imaging technique to detect aldehydes</td>
<td>NOGO: IR signature not detected</td>
</tr>
<tr>
<td>March 2019</td>
<td><strong>Cavitation Modeling:</strong> Differences in cavitation characteristics for different MCCI fuels characterized.</td>
<td>60% complete (awaiting properties for MCCI fuels)</td>
</tr>
<tr>
<td>June 2019</td>
<td><strong>Oxy Fuels &amp; Cold Start:</strong> Complete initial thermodynamic/UHC emissions assessment of three oxygenated blendstocks</td>
<td>On track</td>
</tr>
<tr>
<td>June 2019</td>
<td><strong>CN and Cold Start:</strong> Quantify impact of cetane number on exhaust enthalpy under cold-start conditions for bookend fuels</td>
<td>On track</td>
</tr>
<tr>
<td>June 2019</td>
<td><strong>Cavitation Measurements:</strong> X-ray imaging of cavitation intensity and extent in MCCI nozzles with three fuel blends</td>
<td>On track</td>
</tr>
</tbody>
</table>
Approach – CN, Oxygenates, and Cold Start

- MCCI cold-start strategies use retarded post injection to increase exhaust temperature and quickly reach catalyst light-off – limited by NOx/HC emissions
- Modest increase in cetane number (CN) has been shown\(^1\) to allow increase of exhaust temperature within emissions constraints
- CN approach: explore limits of this strategy with high-CN renewable diesel on a multi-cylinder, heavy-duty MCCI engine platform (ORNL) – directly applicable to new CARB emissions regulations (0.02 g/bhp-hr NOx)
  - Do the benefits of increasing CN continue proportionally or reach point of diminishing return?
  - Can further increases in exhaust temperature be made without increasing NOx/HC emissions?
  - Does high-CN fuel with late post create any unburned or partially-oxidized species that affect catalyst performance?
- Oxygenate approach: thermal, emissions, and optical measurements in a single-cylinder swirl-supported diesel engine (SNL) using three different oxygenate blends with certification diesel
  - Are oxygenated blendstocks able to decrease pollutant emissions for a given exhaust temperature or enable later post injection combustion phasing?

Accomplishments: CN and Cold Start

- Engine platform and experimental hardware selected
  - Multi-cylinder Detroit DD15, 139 mm bore size representative of segment
  - Open ECU architecture: full control of common rail and injections
  - Instrumented cylinder head for combustion analysis
  - FID for total HC emissions, FTIR for detailed speciation
- Fuels have been selected and acquired
  - Low CN fuel: US 2007 Certification Diesel
    - ~46 CN, 178-337 °C boiling range
  - High CN fuel: Paraffinic Renewable Diesel
    - ~75 CN, 189-309 °C boiling range
- Facilities upgrade required to maintain cold-start conditions specified by ACEC Tech Team (20 °C coolant and oil)
  - Chiller has been specified and requisitioned
  - Facilities expected to be fully operational in April
- On track to perform experiments to quantify impact of cetane number on exhaust enthalpy under cold-start conditions in FY19
Accomplishments: Oxy Fuels and Cold Start

- Thermodynamic and exhaust HC emissions measurements have been completed for post injection timing sweeps with three oxygenated blends:
  - OME blend, dibutyl ether, and 1-octanol splash blended with cert diesel

- Oxygenated additives can significantly reduce total hydrocarbon emissions
  - Ethers do this more effectively than 1-octanol

- Oxygenated additives affect the ignition and combustion of the pilot and main injections, but the impact on the post combustion depends on post injection timing
  - The combustion of late post injections is not significantly affected by post injection timing
  - Preliminary evidence: changing fuel composition may not promote robust ignition of late posts

!!! Polyoxymethylene dimethyl ethers (OME) !!!
H₃C
\[ \begin{array}{c}
\text{O} \\
\text{n}
\end{array} \]
\[ \begin{array}{c}
\text{CH₃}
\end{array} \]
OME blend: n=3-5

!!! Dibutyl ether (DBE) !!!
\[ \begin{array}{c}
\text{O}
\end{array} \]
\[ \begin{array}{c}
\text{C₈H₁₈O}
\end{array} \]
CN: ~105

!!! 1-octanol (OCT) !!!
\[ \begin{array}{c}
\text{OH}
\end{array} \]
\[ \begin{array}{c}
\text{C₈H₁₈O}
\end{array} \]
CN: 37

!!! Cert diesel !!!
CN: 43.9

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- Engine speed: 1500 rpm
- \( \text{[O₂]}: 18.4\% \)
- \( \text{Intake: 49 °C} \)
- Pilot-main post: 2-3-4 mg
- Start of pilot injection: 14.5 CAD BTDC
- Start of main injection: TDC
- Start of post injection: 10-30 CAD ATDC

- Retard post injection: heat release rate at start of post decreases

- Oxygenated fuels decrease total hydrocarbon emissions

- Fuel composition impacts combustion of early posts

- Fuel composition effects are diminished for late posts
Approach: Cavitation Modeling

- Fuel property effects on cavitation and erosion are tested using a suite of techniques with varying levels of fidelity and complexity
  - Erosion propensity and severity assessed using model developed at Argonne within the DOE Core Program\(^1\) and validated for single pure fuel\(^2\)
  - Local sensitivity analysis used to identify influential fluid properties
  - Pure fuels of interest tested in geometries of varying complexity:

1. S. Som AMR Presentation: acs075_som_2018
Erosion Propensity has been Predicted for Several Fuels

- Simulations in the throttle geometry were used as an initial fuel screening tool to assess their relative cavitation and erosion propensity.
- Comparison of MCCI and SI fuels with baseline fuels:
  - n-dodecane
  - hexadecane
  - methyl decanoate (MD)
  - undecane
  - iso-octane
  - ethanol
- Variance-based sensitivity analysis\(^1\) of cavitation and erosion predictions to selected liquid fuel properties revealed strong dependencies on liquid density and dynamic viscosity, respectively.
- For pure fuels, the predicted erosion severity ranking was found to be negatively correlated with the liquid dynamic viscosity.

<table>
<thead>
<tr>
<th>Predicted Erosion Severity Ranking</th>
<th>Fuel</th>
<th>(\mu = \mu(T = 330~K)) [Pa-s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>iso-octane</td>
<td>3.26E-04</td>
</tr>
<tr>
<td>2</td>
<td>n-dodecane</td>
<td>8.52E-04</td>
</tr>
<tr>
<td>3</td>
<td>ethanol</td>
<td>6.16E-04</td>
</tr>
<tr>
<td>4</td>
<td>undecane</td>
<td>6.99E-04</td>
</tr>
<tr>
<td>5</td>
<td>methyl decanoate</td>
<td>1.12E-03</td>
</tr>
<tr>
<td>6</td>
<td>hexadecane</td>
<td>1.66E-03</td>
</tr>
</tbody>
</table>

There is some understanding of how fuel properties (esp. vapor pressure) effect cavitation, but almost no work is available on erosion.

Fuels with lower vapor pressure may lead to more severe erosion:
- Enhanced cavitation
- Higher intensity pressure waves at bubble collapse

Two areas of investigation:
- **Measurements of cavitation:** Fundamental measurements of how fuel properties affect cavitation
- **Measurements of erosion:** Measurements of nozzle erosion and the effect of fuel properties
Accomplishments: Cavitation Measurements

- Recent measurements imaged flow separation in the “Spray C” nozzle.
- Studied cavitation intensity and extent for three fuels with a range of vapor pressures.
- Flow is similar between iso-octane and n-dodecane.
- Hexadecane shows weaker, less-defined flow separation layer.
  - Lower vapor pressure, higher viscosity.
  - Cavitation is more dynamic.
  - Dynamics may impact fuel spray distribution, combustion.
- Fuel effects on cavitation measured under realistic conditions for the first time.

\[ P_{\text{inj}} = 1500 \text{ bar}, \quad P_{\text{amb}} = 20 \text{ bar} \]
Accomplishment: Cavitation Modeling & Expt

Measurements and Predictions of Show Good Agreement

**n-dodecane**

Simulations of ECN Spray C showed a Gas Volume Fraction distribution that is comparable to that found in x-ray experiments and can help explaining its nature and composition.

X-ray flow tomography data of **n-dodecane** injection at 1500 bar

**Methyl-decanoate**

LES simulations performed with fixed maximum needle lift

Large velocity and mass flow rate differences (10%) due to different fuel properties

Gas volume fraction is similar at quasi-steady-state flow conditions
All four projects are new in FY 2019, and were not reviewed last year.
Collaboration and Coordination with Other Institutions

- **CN and Cold Start**
  - Daimler, Ford: Technical discussions and support
  - Neste: Renewable diesel

- **Oxy Fuels and Cold Start**
  - Ford Motor Company: regular meetings and teleconferences to discuss experimental approach and results

- **Cavitation Simulations**
  - Argonne: Experimental team and Leadership Computing Facility
  - Univ. Central Florida, NREL: fuel physical properties
  - Univ. of Perugia: Collaboration on Spay C simulations

- **Cavitation Measurements**
  - Argonne: Simulations team and Advanced Photon Source
  - Sandia, Engine Combustion Network: Injectors for study, choice of operating conditions, dissemination of results
• **CN and Cold Start**
  – Current approach with two “bookend” fuels does not indicate if trend is linear or has antagonistic or synergistic behavior at intermediate CN or fuel blend levels
  – Need to translate impact of exhaust enthalpy and emissions under cold-start conditions to light-off performance of diesel oxidation catalyst

• **Oxy Fuels and Cold Start**
  – Need a mechanistic understanding of how oxygenated components impact mixture formation, ignition, and combustion processes to enable cleaner cold start operation

**Cavitation Simulations**
  – There is limited availability of experimental data to characterize multiphase flow development and erosion severity for a range of fuels, especially in practical geometries. Collaborating with experimentalists who can provide such data is critical to validating and informing paths towards predictive fuel screening tools

• **Cavitation Measurements**
  – Running injectors for extended erosion tests is not practical at Argonne. Need to find a partner who can assist us with this task.
Proposed Future Research

• **CN and Cold Start**
  – Experiments will use *blends* of the “bookend” fuels, other high-CN fuels to identify non-linearity or diminishing returns in CN trends for exhaust enthalpy and engine-out emissions
  – Use measured exhaust species concentrations as input conditions for bench-flow reactor study of impact of CN and diesel oxidation catalyst light-off performance. Distribute results through CLEERS.

• **Oxy Fuels and Cold Start**
  – In-cylinder high-speed liquid and vapor-phase fuel imaging, natural luminosity imaging to understand oxygenate impacts on mixture formation, ignition, and combustion

• **Cavitation Simulations**
  – Complete simulation of pure fuels in research nozzle, validate with x-ray experiments
  – Extend screening tool to evaluate cavitation, erosion of fuel *blends*, with blending limit guidelines.
  – Evaluate *multi-hole* injectors, increase fidelity using HPC and Argonne-developed best practices

• **Cavitation Measurements**
  – The cavitation simulations group has requested measurements using methyl decanoate because of its predicted low propensity for erosion. Future measurements will attempt to validate this.
  – Measurements of erosion in a canonical nozzle geometry, establishing the link between fuel properties and erosion rates.

*Any proposed future work is subject to change based on funding levels*
• **CN and Cold Start**
  – Cetane number (CN) is an important fuel property for MCCI as it can dictate how aggressively the post injections can be retarded for quick catalyst warm-up during cold-start. This task will quantify the effect of high-CN fuel on engine-out exhaust enthalpy and emissions under cold-start conditions.

• **Oxy Fuels and Cold Start**
  – Oxygenated fuels reduce total hydrocarbon emissions in MCCI catalyst heating operation, but further study is needed to understand their impact on the ignition of late post injections

• **Cavitation Simulations**
  – Computational screening tool for pure fuels identified trends relating fuel properties to cavitation, and flagged fuels with increased propensity for cavitation and erosion

• **Cavitation Measurements**
  – Measurements have found variations in cavitation with fuel properties. The measurement results will be shared with the simulations group to validate their work.